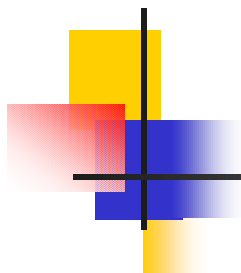


TOXNET

Toxicology and Environmental Health Information

from the National Library of Medicine (NLM)

and Other Sites



Presented by

NLM's Toxicology and Environmental Health Information Program

part of the Division of Specialized Information Services

Contact:

Toxicology and Environmental Health Information Program

Division of Specialized Information Services

National Library of Medicine

Suite 510, MSC 5467

6707 Democracy Blvd.

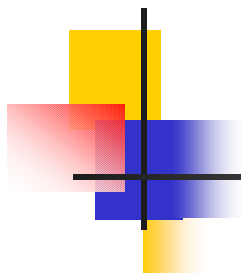
Bethesda, MD 20892-5467

301-496-1131

301-480-3537 (FAX)

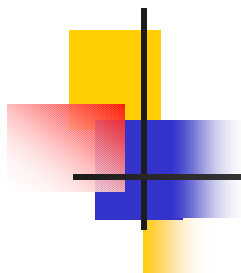
Web site: <http://sis.nlm.nih.gov/>

Contact: tehip@tehl.nlm.nih.gov



Class Schedule

Part I	Overview of NLM Tox Resources	9:00 - 9:30
Part II	TOXNET Overview, HSDB & Related Files	9:30 - 10:30
	<i>Break</i>	10:30 - 10:45
Part III	TOXLINE and Related Files	10:45 - 11:30
	<u>Practicum</u>	11:30 - 12:15
	<i>Lunch</i>	12:15 - 1:30
Part IV	TRI and other Specialty Files	1:30 - 2:15
Part V	Non-NLM Resources	2:15 - 3:00
	<i>Break</i>	3:00 - 3:15
Part VI	ChemIDplus	3:15 - 3:45
	<u>Practicum</u>	3:45 - 4:30



Part I

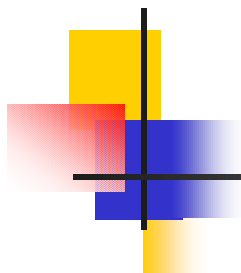
An Overview of Toxicology and Environmental Health Information Resources at the National Library of Medicine



Toxicology and Environmental Health Information Program (TEHIP)

Background

- ✍ Poisons recognized throughout time.
- ✍ Socrates - hemlock. Cleopatra - asp.
- ✍ Harvey W. Wiley's Poison Squad – 1903
- ✍ The Jungle (1906) Upton Sinclair – lack of hygiene in the meat-packing industry
- ✍ Food and Drugs Act (1906) – prohibited adulterated or misbranded items
- ✍ Federal Food, Drug and Cosmetic Act (1938) – enhanced safety requirements for drugs
- ✍ Drug Amendments (1962) – effectiveness required for drugs
- ✍ Silent Spring (1962) Rachel Carson – sparked public awareness about hazards of synthetic chemicals
- ✍ President's Science Advisory Committee (1966) – “Report on the Handling of Toxicological Information”
- ✍ TEHIP Created (1967)
- ✍ Situated within NLM's Division of Specialized Information Services

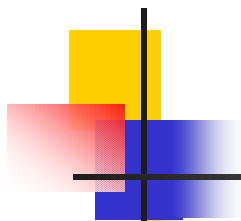


TEHIP Mission

- ✍ Provide selected core toxicology and environmental health information resources and services
- ✍ Facilitate access to national and international toxicology and environmental health information resources
- ✍ Strengthen the information infrastructure of toxicology and environmental health

So...TEHIP

- ✍ Builds and/or makes available free online Web-based databases
- ✍ Creates other Web-based resources
- ✍ Collaborates with government agencies and others
- ✍ Is active in public training and outreach



TEHIP Databases

- ✍ TOXNET System of Databases (including ChemID*plus* and Specialty Databases)
- ✍ DIRLINE (directory of organizations)

Additional TEHIP Resources

- ✍ Special Topic Guides – arsenic, biological & chemical warfare agents, etc.
- ✍ Publications (including Glossary of Terms Used in Toxicology)
- ✍ ALTBIB - Alternatives Bibliography
- ✍ Toxicology Tutor

Other Relevant NLM Information

- ✍ PubMed/MEDLINE
- ✍ MEDLINE*plus* (consumer health, includes drug information)
- ✍ Clinical Trials
- ✍ NLM Gateway – Multi-File Searching – Planned to go across all NLM Files



About

The Specialized Information Services (SIS) Division of the National Library of Medicine (NLM) is responsible for information resources and services in toxicology, environmental health, chemistry, HIV/AIDS, and specialized topics in minority health.



Toxicology & Environmental Health

Databases and other resources related to toxicology and environmental health. Features [TOXNET](#).



Chemical Information

Databases and other resources designed to help you search for information by chemical name or structure. Features [ChemIDplus](#).



HIV / AIDS

Links to journal literature, clinical trials and treatment information, meeting abstracts, and other scientific and consumer-related resources.



Directory of Health Organizations

Features [DIRLINE](#) and [Health Hotlines](#).

More to Explore

[News](#)
[Outreach Activities](#)
[Staff Directory](#)
[Site Map and Search](#)

**Environmental Justice
Internet Guide** NEW

**Asian American Health
Web Site** NEW

AIDSinfo

Tox Town

Your health, toxic substances, and the environment.

Other NLM Resources

[NLM Gateway](#) search
multiple NLM databases
[MEDLINE/PubMed](#) search
journal literature
[LOCATORplus](#) books,
journals, audiovisuals



Toxicology and Environmental Health

TOXNET

Databases in toxicology and environmental health.

TOXLINE	HSDB	ChemIDplus
DART	TRI	IRIS
GENE-TOX	CCRIS	

Internet Resources

Evaluated links to Internet resources on current issues such as [chemical warfare agents](#) and [Environmental Justice](#).

Haz-Map

Database on hazardous chemicals and occupational diseases.

ALTBIB

References about alternatives to the use of live animals in biomedical research and testing.

Toxicology Tutor

Three self-guided tutorials on toxicology.

News and Events

Links to news items on the web site, [outreach activities](#) and a [calendar of events](#).

Consumer Health

Tox Town

An interactive guide to commonly encountered toxic substances.

MEDLINEplus

[Poisoning, Toxicology and Environmental Health](#)

DIRLINE

Over 10,000 health organizations.

Health Hotlines

Toll-free numbers to 300 organizations.

MEDLINE/PubMed

References from more than 4,600 biomedical journals, including the [Toxicology Subset](#).

Other Resources

Chemical Information

Selected Toxicology Links

- [10th Report on Carcinogens](#) (National Toxicology Program)
- [Second National Report on Human Exposure to Environmental Chemicals](#) (Centers for Disease Control and Prevention)

Reference Material

Bibliographies, glossary, reports.

Database descriptions

TOXNET Manual

Locatorplus

The NLM catalog of books, journals, and audiovisuals.

NLM Gateway

Search multiple databases at NLM.



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Specialized Information Services

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SIS



Directory of Health Organizations Online

► [Directory of Health Organizations](#) ►

DIRLINE

[Search DIRLINE](#)

[Other NLM Resources](#)

Search:

☒ all of the words ☐ any of the words ☐ exact phrase

Fields: (if none checked, all fields will be searched.)

☐ Organization name or acronym

☐ MeSH Headings/Keywords

Select records containing:

☐ Only organizations with toll-free numbers

☐ Only organizations with services for the hearing impaired

[Health Hotlines](#)

[MEDLINEplus](#)

[PubMed](#)

[NLM Gateway](#)

[Locatortplus](#)

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Customer Service: tehip@tehl.nlm.nih.gov

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DIRLINE Search Results

[Directory of Health Organizations](#)

[DIRLINE](#)

Save
Checked Items

Sort

Details

History

Download

Modify Search

New Search

Browse Index

SIS
Home

MEDLINEplus
Home

drinking water

Search

Clear

Items 1 through 20 of 49

Pages: [1](#) [2](#) [3](#) ▶

Organization Names are sorted in [relevancy ranked](#) order.

Select Record	Organization Name
1 <input type="checkbox"/>	Drinking Water Program - Massachusetts Department of Environmental Protection
2 <input type="checkbox"/>	National Drinking Water Clearinghouse - Environmental Services and Training Division - West Virginia University (NDWC)
3 <input type="checkbox"/>	Office of Water Quality - Indiana Department of Environmental Management
4 <input type="checkbox"/>	U.S. Environmental Protection Agency - Office of Research and Development - National Risk Management Research Laboratory - Water Supply and Water Resources Division
5 <input type="checkbox"/>	Office of Drinking Water Quality - Rhode Island Department of Health
6 <input type="checkbox"/>	American Water Works Association (AWWA)
7 <input type="checkbox"/>	Office of Water, U.S. Environmental Protection Agency (OW)
8 <input type="checkbox"/>	WATERNET - American Water Works Association - Information Services
9 <input type="checkbox"/>	Drinking Water Program - Drinking Water and Environmental Management Division - California Department of Health Services
10 <input type="checkbox"/>	Water Environment Federation (WEF)
11 <input type="checkbox"/>	Clean Water Action (CWA)
12 <input type="checkbox"/>	Nevada Department of Human Resources - Division of Health - Bureau of Health Protection Services
13 <input type="checkbox"/>	Kentucky Natural Resources and Environmental Protection Cabinet - Department for Environmental Protection - Division of Water
14 <input type="checkbox"/>	Maine Department of Human Services - Division of Health Engineering (MEDHE)
15 <input type="checkbox"/>	Environmental Health Services - Fulton County Board of Health
16 <input type="checkbox"/>	International Office For Water - Office International de L'Eau
17 <input type="checkbox"/>	American Water Resources Association (AWRA)
18 <input type="checkbox"/>	New England Water Works Association (NEWWA)


Search

[Home](#) | [About](#) | [Site Map](#) | [FAQs](#) | [Contact Us](#)

[español](#)

Health Topics [Drug Information](#) [Encyclopedia](#) [Dictionary](#) [News](#) [Directories](#) [Other Resources](#)

Poisoning, Toxicology, Environmental Health Topics

- [Air Pollution](#)
- [Anthrax](#)
- [Arsenic](#)
- [Asbestos/Asbestosis](#)
- [Biodefense and Bioterrorism](#)
- Biological Weapons see [Biodefense and Bioterrorism](#)
- Bioterrorism see [Biodefense and Bioterrorism](#)
- Campylobacter see [Food Contamination/Poisoning](#)
- [Carbon Monoxide Poisoning](#)
- Cell Phones see [Electromagnetic Fields](#)
- [Chemical Weapons](#)
- Cleaning Products see [Household Poisons](#)
- [Drinking Water](#)
- EMF see [Electromagnetic Fields](#)
- [Electromagnetic Fields](#)
- [Environmental Health](#)
- Environmental Tobacco Smoke see [Secondhand Smoke](#)
- [Food Contamination/Poisoning](#)
- [Food Safety](#)
- Fungicides see [Pesticides](#)

[Browse](#) : [By Condition](#) : [By Disease Heading](#) : [Injuries, Poisonings, and Occupational Diseases](#) : **Disorders of Environmental Origin**

☐ **Show all trials, including those no longer recruiting patients.**

Click on title to see details. Or, select multiple checkboxes and press "Display Selected Studies" at bottom of page.

150 studies were found. Here are studies 1 to 50. [Next 50](#)

1. ☐ **Recruiting** [Reducing Pesticide Exposure in Minority Families](#)
Condition: Disorders of Environmental Origin
2. ☐ **Recruiting** [Does Lead Burden alter Neuropsychological Development?](#)
Condition: Lead Poisoning
3. ☐ **Recruiting** [Cocaine Effects in Humans: Physiology and Behavior](#)
Condition: Cocaine-Related Disorders
4. ☐ **Not yet recruiting** [Pharmacological Modulation of Cocaine Effects](#)
Condition: Cocaine-Related Disorders
5. ☐ **Recruiting** [IV Cocaine Abuse: A Laboratory Model](#)
Condition: Cocaine-Related Disorders
6. ☐ **Recruiting** [Combined Buprenorphine and Behavioral Tx w/out contingent reinforcement](#)
Conditions: Cocaine-Related Disorders; Opioid-Related Disorders
7. ☐ **Recruiting** [Flupenthixol Decanoate in Methamphetamine Smoking](#)
Condition: Substance-Related Disorders
8. ☐ **Recruiting** [Evaluation of Opioid Antagonist Activity in Humans](#)
Condition: Opioid-Related Disorders
9. ☐ **Recruiting** [Evaluation of a Desipramine Ceiling in Cocaine Abuse](#)
Conditions: Substance-Related Disorders; Cocaine-Related Disorders
10. ☐ **Not yet recruiting** [Risperidone Treatment in Dually-Diagnosed Individuals](#)
Condition: Cocaine-Related Disorders
11. ☐ **Recruiting** [Cocaine Abuse and Attention Deficit Disorder](#)
Condition: Cocaine-Related Disorders
12. ☐ **Recruiting** [Pergolide Treatment for Substance Abusers](#)
Conditions: Substance-Related Disorders; Cocaine-Related Disorders



Gateway

your entrance to the
knowledge resources of the
National Library of Medicine

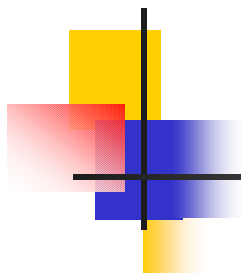
[Search](#)[Clear
Search](#)[Find Terms](#)[Limits](#)[Results](#)[History](#)[Locker](#)[Preferences](#)

New Search

[Overview](#)[What's New](#)[Help](#)[F A Q](#)[Other NLM
Resources](#)[Ordering Info.](#)[Clinical Alerts](#)[ClinicalTrials.gov](#)[HSTAT](#)[LOCATORplus](#)[MEDLINEplus](#)[PubMed](#)[TOXNET](#)

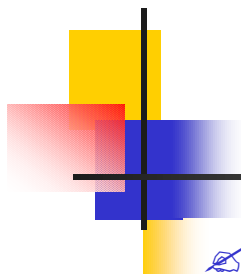
Results Summary

Category	Items Found	Actions	
Journal Citations	2125	Display Results	Details of Search
Books / Serials / AVs	25	Display Results	Details of Search
Consumer Health	12	Display Results	Details of Search
Meeting Abstracts	3	Display Results	Details of Search
Other Collections	5	Display Results	Details of Search
Total	2170		



Part II

TOXNET Overview, HSDB, & Related Files



What is TOXNET?

- ✍ A free web-based system of databases on toxicology, environmental health, hazardous chemicals, toxic releases, chemical nomenclature, and specialty areas such as occupational health and consumer products
- ✍ A product of NLM's Toxicology and Environmental Health Information Program
- ✍ Toxicology Data (one record per chemical)– HSDB, IRIS, CCRIS, GENE-TOX (can also search any combination of these files with “Multi-Databases” interface)
- ✍ Toxicology Literature (bibliographic references) – TOXLINE, DART/ETIC
- ✍ Toxic Releases (of chemicals to the environment) – TRI
- ✍ Chemical Identification/Nomenclature – ChemIDplus
- ✍ Specialty Databases – HazMap, Consumer Products (planned)
- ✍ User Support – tehip@the.nlm.nih.gov or click on “Contact TOXNET”

Where is TOXNET?

toxnet.nlm.nih.gov



TOXNET

► [Tox. & Env. Health](#) ► [TOXNET](#)

Welcome to TOXNET, a cluster of databases on toxicology, hazardous chemicals, and related areas.

Databases

HSDB	i
IRIS	i
GENE-TOX	i
CCRIS	i
Multi-Databases	i
TOXLINE	i
DART/ETIC	i
TRI	i
ChemIDplus	i



Need More
Information?

Search All Databases

Search

Clear

Other NLM Resources

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[Haz-Map](#)
[AltBib](#)
[Tox Weblinks](#)
[MEDLINEplus](#)
[Tox/Env. Health subset](#)
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SIS



TOXNET

► [Tox. & Env. Health](#) ► [TOXNET](#)

Welcome to TOXNET, a cluster of databases on toxicology, hazardous chemicals, and related areas.

Databases

HSDB	i
IRIS	i
GENE-TOX	i
CCRIS	i
Multi-Databases	i
TOXLINE	i
DART/ETIC	i
TRI	i
ChemIDplus	i



Need More
Information?

Search All Databases

Other NLM Resources

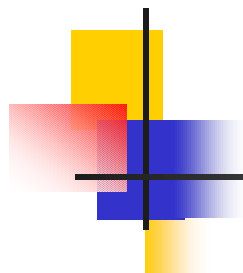
[DIRLINE](#)
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[AltBib](#)
[Tox Weblinks](#)
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Toxicology Data Files - Content

Hazardous Substances Data Bank (HSDB) – from NLM

4671 Chemical Records

Human Health Effects

Emergency Medical Treatment

Animal Toxicity Studies

Metabolism/Pharmacokinetics

Pharmacology

Environmental Fate/Exposure

Environmental Standards & Regulations

Chemical/Physical Properties

Chemical Safety & Handling

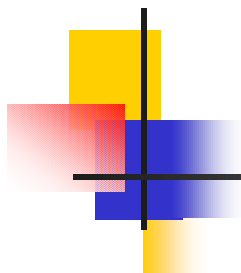
Occupational Exposure Standards

Manufacturing and Use

Laboratory Methods

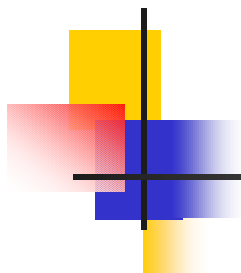
Special References

Synonyms and Identifiers



More about HSDB

- ✍ Factual Data Bank/Online Handbook
- ✍ Peer-Reviewed – Scientific Review Panel
- ✍ Review Status Tags – Peer Reviewed, QC Reviewed, Unreviewed
- ✍ Fully Referenced
- ✍ Data – Excerpted from books, government documents, technical reports, selected primary literature, databases. Some data compiled expressly for HSDB.



Toxicology Data Files - Content

Chemical Carcinogenesis Research Information System (CCRIS) –
from the National Cancer Institute (NCI)
8868 Chemical Records

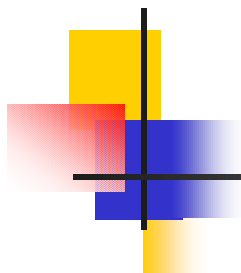
Carcinogenicity Studies

Tumor Inhibition Studies

Tumor Promotion Studies

Mutagenicity Studies

e.g. Carcinogenicity Studies Data Structure – species, route, tumor site/type of lesion, results, reference



Toxicology Data Files - Content

GENE-TOX

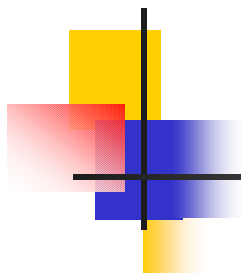
from the U.S. Environmental Protection Agency (EPA)

3214 Chemical Records

Note: GENE-TOX not updated since January 2000

Mutagenicity Studies

Data Structure – assay type, assay code, results, panel report, reference



Toxicology Data Files - Content

Integrated Risk Information System (IRIS) from the U.S. Environmental Protection Agency (EPA) 538 Chemical Records

Noncarcinogenic Assessment – Oral (RfD) Carcinogenic Assessment - Oral

Noncarcinogenic Assessment – Inhalation (RfC) Carcinogenic Assessment -
Inhalation

- ✍ Contains EPA consensus scientific positions and quantitative values on cancer and non-cancer health effects that may result from lifetime oral or inhalation exposure to specific chemical substances in the environment
- ✍ Risk Assessment – Identification and quantification of risk. Function of toxicity and exposure
- ✍ Risk Assessment Process (National Academy of Sciences, 1983) – 1. Hazard identification, 2. Dose-Response assessment [IRIS], 3. Exposure assessment, 4. Risk Characterization



TOXNET Search Screen Options

- ✍ TOXNET Home Page Search

- ✍ Single query box search

- ✍ No limits

- ✍ Gives quick counts of records retrieved and allows links to each database

- ✍ Number of records retrieved in each database may vary from numbers attained by searching databases directly



- ✍ Database specific searches – interface varies according to type of database

- ✍ Multi-Databases search – interface for any combination of data files (i.e. HSDB, CCRIS, GENE-TOX, IRIS)






Search Page - Toxicology Data Files

One Box Search for:

-  Chemicals – enter chemical names or CAS Registry numbers.
Let system add synonyms (default) or use exact terms entered.
-  Other Terms

Browse Index for:















-  All Words
-  Chemical name
-  CAS Registry Number

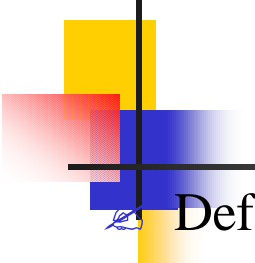
Limits

-  For more precise searching – searching for terms within particular data fields



Search Results Page -Toxicology Data Files

-  Displays chemical names and registry numbers of retrieved records
-  Relevancy Ranked Display
-  Select Record(s) of Interest
-  View Details of Search Strategy
-  Modify Search – Returns you to Search Page with query intact
-  Begin a New Search – Returns you to Search Page with blank query box
-  Or Search can be modified or begun anew directly on Results Page
-  Sort Results – By substance name, ascending or descending sequence
-  Save Checked Items, Display Checked Items
-  View Search History and combine search statements
-  Download – Entire Record(s) or Custom Format
-  Browse Index
-  Get Help
-  Return to TOXNET Home



Selected Record Page - Toxicology Data Files

 Default display varies

 Chemical Search – HSDB displays human health effects, other files display full record


 Other Term(s) Search – Best Sections


 **Search Term(s) Highlighted in Red**

 Choose fields for display from Contents (expand, contract categories)

 Navigate – Next Item, Previous Item

 View Details of Search Strategy

 Modify Search – Returns you to Search Screen with query intact


 Begin a New Search – Returns you to Search Screen with blank query box

 Download – Entire Record(s) or Custom Format

 Browse Index

 Get Help

 Return to TOXNET Home

 Link to records for the same chemical in Other Files - (including TOXLINE and ChemID*plus*)



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SIS



Hazardous Substances Data Bank

▶ [Tox. & Env. Health](#) ▶ [TOXNET](#) ▶ [HSDB](#)

Databases

Hazardous Substances Data Bank	i
IRIS	i
GENE-TOX	i
CCRIS	i
Multi-Databases	i
TOXLINE	i
DART/ETIC	i
TRI	i
ChemIDplus	i
TOXNET Home	

Search HSDB

acetone

Search

Clear

For chemicals, add synonyms
and CAS numbers to search:

☒ Yes ☐ No

Limits

Browse the Index

Other NLM Resources

[DIRLINE](#)

[Haz-Map](#)

[AltBib](#)

[Tox Weblinks](#)

[MEDLINEplus](#)

[Tox/Env. Health subset](#)

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[Sample Record](#)

[HSDB Scientific Review
Panel](#)

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HSDB Search Results

[Tox. & Env. Health](#) [TOXNET](#) [HSDB](#)

- Save Checked Items
- Sort
- Details
- History
- Download
- Modify Search
- Basic Search
- Browse Index
- Help
- TOXNET Home

acetone

Search

Clear

Limits

For chemicals, add synonyms and CAS numbers to search: ☒ Yes ☐ No

Items 1 through 20 of 1878

Page 1 of 94. to page

Substance Names are sorted in [relevancy ranked](#) order.

Select Record	Substance Name
---------------	----------------


The following is the primary record for the chemical. All of the query terms were found.

- | | |
|----------------------------|------------------------------------|
| 1 <input type="checkbox"/> | ACETONE
67-64-1 |
|----------------------------|------------------------------------|

The following 1877 records contain one or more of the requested chemical name(s) and all of the query terms anywhere in the record.

- | | |
|----------------------------|--|
| 2 <input type="checkbox"/> | ACETONE CYANOHYDRIN
75-86-5 |
| 3 <input type="checkbox"/> | 1-CHLORO-2-PROPANONE
78-95-5 |
| 4 <input type="checkbox"/> | ISOPROPANOL
67-63-0 |
| 5 <input type="checkbox"/> | 1,1,1,3,3,3-HEXAFLUORO-2-PROPANONE
684-16-2 |
| 6 <input type="checkbox"/> | ACETONITRILE
75-05-8 |
| 7 <input type="checkbox"/> | METHYL ETHYL KETONE
78-93-3 |
| 8 <input type="checkbox"/> | ACETYL ACETONE
123-54-6 |

Contents

Contract all categories Expand all categories 

Select

Clear

- ☐  [FULL RECORD](#)
- ☒  [Human Health Effects](#)
- ☒  [Emergency Medical Treatment](#)
- ☒  [Animal Toxicity Studies](#)
- ☒  [Metabolism/Pharmacokinetics](#)
- ☒  [Pharmacology](#)
- ☒  [Environmental Fate & Exposure](#)
- ☒  [Environmental Standards & Regulations](#)
- ☒  [Chemical/Physical Properties](#)
- ☒  [Chemical Safety & Handling](#)
- ☒  [Occupational Exposure Standards](#)
- ☒  [Manufacturing/Use Information](#)
- ☒  [Laboratory Methods](#)
- ☒  [Special References](#)
- ☒  [Synonyms and Identifiers](#)
- ☒  [Administrative Information](#)


ACETONE

CASRN: 67-64-1

*For other data, click on the Table of Contents***Human Health Effects:****Toxicity Summary:**

Exposure to **acetone** results from both natural and anthropogenic sources. **Acetone** also occurs as a metabolic component in blood, urine and human breath. ... **Acetone** is one of three ketone bodies that occur naturally throughout the body. It can be formed endogenously in the mammalian body from fatty acid oxidation. Fasting, diabetes mellitus and strenuous exercise increase endogenous generation of **acetone**. Under normal conditions, the production of ketone bodies occurs almost entirely within the liver and to a smaller extent in the lung and kidney. ... Products are excreted in the blood and transported to all tissues and organs of the body where they can be used as a source of energy. Two of these ketone bodies, acetoacetate and beta-hydroxybutyrate, are organic acids that can cause metabolic acidosis when produced in large amounts, as in diabetes mellitus. ... Endogenous **acetone** is eliminated from the body either by excretion in urine and exhaled air or by enzymatic metabolism. ... **Acetone** is rapidly absorbed via the respiratory and gastrointestinal tracts of human and laboratory animals, as indicated by the detection of **acetone** in blood within 30 min of inhalation exposure and 20 min of oral administration. ... The nasal cavities of human and laboratory animals appear to have a limited ability to absorb and excrete **acetone** vapor, compared with the remainder of the respiratory tract. **Acetone** is uniformly distributed among non-adipose tissues and does not accumulate in adipose tissue. ... **Acetone** is rapidly cleared from the body by metabolism and excretion. ... Exhalation is the major route of elimination for **acetone** and its terminal metabolite (carbon dioxide), and the fraction of administered **acetone** that is exhaled as unchanged **acetone** is dose-related. Urinary excretion of **acetone** and its metabolites occurs but this route of elimination is minor ... Exogenously supplied **acetone** enters into many metabolic reactions in tissues throughout the body, but the liver appears to be the site of most extensive metabolism. Carbon from orally administered **acetone** has been detected in cholesterol, amino acids, fatty acids and glycogen in rat tissues, urea in urine and unchanged **acetone** and CO₂ in exhaled breath. Metabolically, **acetone** is degraded to acetate and formate ... Oral LD₅₀ values in adult rats are in the range of 5800-7138 mg/kg. ... Experimental animal data characterizing the effects of long term oral or inhalation exposure to **acetone** are not available, due probably to its low toxicity and its

Contents

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- ☐  [Occupational Exposure Standards](#)
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ACETONE

CASRN: 67-64-1

For other data, click on the Table of Contents

Metabolism/Pharmacokinetics:

Metabolism/Metabolites:

Two pathways for the conversion of **acetone** to glucose are proposed, the methylglyoxal & the propanediol pathways. The methylglyoxal pathway is responsible for the conversion to acetol, acetol to methylglyoxal, & subsequent conversion of methylglyoxal to glucose. The propanediol pathway involves the conversion of acetol to L-1,2-propanediol by an as yet unknown process. L-1,2-propanediol is converted to L-lactaldehyde by alcohol dehydrogenase, & L-lactaldehyde is converted to L-lactic acid by aldehyde dehydrogenase. Expression of these metabolic pathways in rat appears to be dependent on the induction of **acetone**/ oxygenase & acetol monooxygenase by **acetone**.

[Casazza JP et al; J Biol Chem 259 (1): 231-6 (1984)]**PEER REVIEWED**

HEPATIC NAD-DEPENDENT ALCOHOL DEHYDROGENASE ... ENZYME IS CAPABLE OF CATALYZING REVERSE REACTION IN WHICH ... **ACETONE** ... /IS REDUCED TO ALCOHOL/.

[Testa, B. and P. Jenner. Drug Metabolism: Chemical & Biochemical Aspects. New York: Marcel Dekker, Inc., 1976. 310]**PEER REVIEWED**

Acetone may be converted to 1,2-propanediol which enters the glycolytic pathway & possibly the one carbon pool. **Acetone** has been shown to be converted to lactate in mice. The rate-limiting step appears to be the conversion of **acetone** to a hydroxylated intermediate. Rats & mice exposed to 30 mg/l of **acetone**, & rabbits & guinea pigs exposed to 72 mg/l for 2 hr, had increased levels of **acetone**, acetoacetic acid, & beta-hydroxybutyric acid in the blood & urine immediately after exposure & 24 hr later.


[Clayton, G. D. and F. E. Clayton (eds.). Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology. 3rd ed. New York: John Wiley Sons, 1981-1982. 4726]**PEER REVIEWED**

Acute admin of **acetone** to rats resulted in measureable levels of isopropanol in blood. Metabolism of **acetone** to isopropanol was different in normal & diabetic animals. Blood levels of isopropanol reached a max at 2 hrs after dose in normal rats, but there was a 2-phase response in diabetic rats. In a

Links to Related Records in Other Database...

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ACETONE

CASRN: 67-64-1

*For other data, click on the Table of Contents***Substance Identification:****Substance Name:** ACETONE**CAS Registry Number:** 67-64-1**Data Type:**

Mutagenicity

Studies Data:**Mutagenicity Studies:**




Test System:	AMES SALMONELLA TYPHIMURIUM
Strain Indicator:	TA100
Metabolic Activation:	NONE
Method:	PREINCUBATION
Dose:	100-10000 UG/PLATE (TEST MATERIAL SOLVENT: DISTILLED WATER)
Results:	NEGATIVE

Reference:

[ZEIGER, E, ANDERSON, B, HAWORTH, S, LAWLOR, T AND MORTELMANS, K; SALMONELLA MUTAGENICITY TESTS. V. RESULTS FROM THE TESTING OF 311 CHEMICALS; ENVIRON. MOL. MUTAGEN. 19 (SUPPL.21):2-141, 1992]

Test System:	AMES SALMONELLA TYPHIMURIUM
Strain Indicator:	TA100
Metabolic Activation:	HAMSTER, LIVER, S-9, AROCLOR 1254 (10 OR 30%)

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Add chemical synonyms and CAS numbers to search:
☒ Yes ☐ No

Search: ☐ exact words ☒ singular & plural forms ☐ word variants
 Search records with: ☐ the phrase ☒ all words ☐ any words

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Search History

- ✍ To review search strategies
- ✍ To combine search statements (within databases)
- ✍ Query Box provided to enter subsequent searches directly on Search History Page
- ✍ Use # to combine search statements (e.g. #1 AND #2)

Search *HSDB* for **#1 AND #2**

- Search History will be lost after one hour of inactivity.
- To combine searches use # before search number. e.g. #2 AND #6.
- Searches may not be combined across databases.

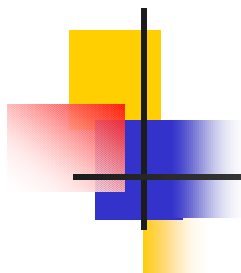
Search	Database	Query	Time	Result
# 2	hsdb	[use] [mfs] [mmnfg] [omin] [form] [imp] [cpat] [prod] [impt] "latex paint" [expt]	10:12:24	19
# 1	hsdb	[tox] [care] [htox] [htxv] [seri] [warn] [meds] [popl] [rtex] [body] [avdi] "lymphatic leukemia" [minf]	10:12:03	5

Clear History



Boolean Searching, Field Qualification, Search Techniques

- ✍ Upper Case Boolean Operators (AND, OR, NOT)
- ✍ Fields in brackets and post-qualified (e.g. benzene [na])
- ✍ Nested parenthesis permitted
- ✍ Phrase searching with quotation marks (e.g. “coronary artery bypass”)
- ✍ Asterisk (*) for truncation (e.g. carcinogen*)



Part III

TOXLINE and Related Files



TOXLINE

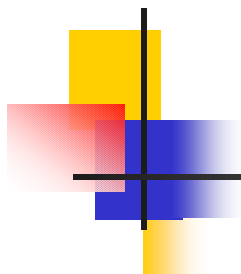
TOXicology Literature onLine

- ✍ Covers pharmacological, biochemical, physiological, environmental, and toxicological effects of chemicals/other agents on living systems
- ✍ Citations, Abstracts, Keywords and/or MeSH (Medical Subject Headings)
- ✍ CAS Registry Numbers
- ✍ From 1965 to date (and earlier)
- ✍ Drawn from Secondary Sources, varying unit record formats
- ✍ Components – TOXLINE Core (on PubMed, accessible via TOXNET) and TOXLINE Special (on TOXNET)
- ✍ Over 3 million toxicology related records combined



TOXLINE Core (on PubMed)

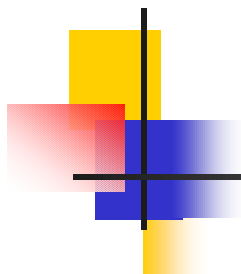
- ✍ Toxicology Subset limit of MEDLINE on PubMed
- ✍ Similar to TOXLINE's former TOXBIB subfile
- ✍ Drawn from standard biomedical journal literature
- ✍ Accessible directly on PubMed or from the TOXLINE search screen on TOXNET
- ✍ Some features of PubMed:
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 - ✍ Limit by field, publication type, age, gender, language, human or animal, etc.
 - ✍ Cubby – to store and update searches
 - ✍ Related articles
 - ✍ LinkOut + Links to Books
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TOXLINE Special (on TOXNET)

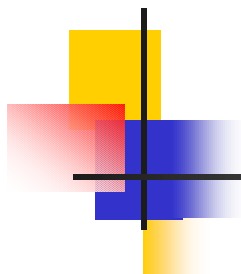
- ✍ Technical Reports and Research projects
 - ✍ Federal Research in Progress (FEDRIP)
 - ✍ Toxicology Document and Data Depository (NTIS)
 - ✍ Toxicology Research Projects (CRISP)
 - ✍ Toxic Substances Control Act Test Submissions (TSCATS)

- ✍ Special Journal and Other Research Literature
 - ✍ Developmental and Reproductive Toxicology (DART)
 - ✍ International Labour Office (CIS)
 - ✍ Swedish National Chemicals Inspectorate (RISKLINE)



TOXLINE Special (continued)

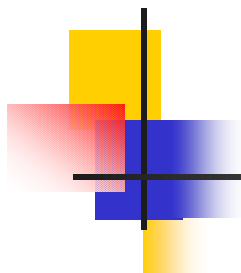
- ✍ Archival Collections (No Longer Being Updated)
 - ✍ Aneuploidy (ANEUPL)
 - ✍ Environmental Mutagen Information Center file (EMIC)
 - ✍ Environmental Teratology Information Center file (ETIC)
 - ✍ Epidemiology Information System (EPIDEM)
 - ✍ Hazardous Materials Technical Center (HMTC)
 - ✍ International Pharmaceutical Abstracts (IPA)
 - ✍ NIOSHTIC (NIOSH)
 - ✍ Pesticides Abstracts (PESTAB)
 - ✍ Poisonous Plants Bibliography (PPIB)
 - ✍ Toxicological Aspects of Environmental Health (BIOSIS)



TOXLINE Special (continued)

- ✍ Some Features of TOXLINE Special
 - ✍ Relevancy Ranking
 - ✍ Toggle between TOXLINE Special and TOXLINE Core
 - ✍ Automatic Mapping to MeSH terms
 - ✍ Link to TOXLINE Special from *ChemIDplus*
 - ✍ Related Articles

Note: Search algorithms and display formats of TOXLINE Special and TOXLINE Core vary.



Another Toxicology Literature File













Developmental and Reproductive Toxicology (DART/ETIC)
100,813 Records

- ✍ Covers Developmental and Reproductive Toxicology (including Teratology)
- ✍ Components – DART Core (on PubMed) and DART Special (on TOXNET)



Search Page - Toxicology Literature Files

One Box Search for:

-  Chemicals – enter chemical names or CAS Registry numbers.
Let system add synonyms (default) or use exact terms entered.
-  Other Terms
-  Select TOXLINE Special, TOXLINE Core or both (default)
-  Browse Index for:
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 -  Authors
 -  MeSH Headings/Keywords
 -  CAS Registry Numbers
-  Automatic Term Mapping to MeSH & UMLS
 -  e.g. passive smoking --- tobacco smoke pollution
-  Limits
 -  For more precise searching – to search within all fields, title only, author only, by specific range of years of publication, subfile, language, etc.



Search Results Page - Toxicology Literature Files

- ✍ Displays title, author, source, subfile of retrieved records
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- ✍ Or Search can be modified or begun anew directly on Results Page
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- ✍ Displays full bibliographic record – Title, Author, Source, Abstract, keywords, etc.
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- ✍ **Hot Linked Items (e.g. authors, keywords, CAS registry numbers) highlighted and underlined, in Blue**
- ✍ Related Records
- ✍ Return to Search Results page
- ✍ Download – Brief, Full, Abstract, Tagged
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brain cancer pesticide

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brain cancer pesticides

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- 1 ☐ [Pesticide Prioritization for a Brain Cancer Case-Control Study](#)
Sanderson WT ; Talaska G ; Zaebs D ; Davis-King K ; Calvert G
Environmental Research, Vol. 74, No. 2, pages 133-144, 28 references, 1997 [NIOSH]
- 2 ☐ [Pesticide prioritization for a brain cancer case-control study.](#)
SANDERSON WT ; TALASKA G ; ZAEBST D ; DAVIS-KING K ; CALVERT G
ENVIRONMENTAL RESEARCH; 74 (2). 1997. 133-144. [BIOSIS]
- 3 ☐ [Occupational Risk Factors for Brain Tumors among Women in Shanghai, China](#)
Heineman EF ; Gao Y-T ; Dosemeci M ; McLaughlin JK
Journal of Occupational and Environmental Medicine, Vol. 37, No. 3, pages 288-293, 22 references, 1995 [NIOSH]
- 4 ☐ [Brain cancer mortality among French farmers: The vineyard pesticide hypothesis.](#)
VIEL J-F ; CHALLIER B ; PITARD A ; POBEL D
ARCHIVES OF ENVIRONMENTAL HEALTH; 53 (1). 1998. 65-70. [BIOSIS]
- 5 ☐ [Family pesticide use and childhood brain cancer.](#)
DAVIS JR ; BROWNSON RC ; GARCIA R ; BENTZ BJ ; TURNER A
ARCH ENVIRON CONTAM TOXICOL; 24 (1). 1993. 87-92. [BIOSIS]
- 6 ☐ [Occupational exposures in spraying and application of insecticides](#)
IARC working group
TA:IARC Monographs on the evaluation of the carcinogenic risk of chemicals to humans PG:45-92 YR:1991 IP: VI:53 [RISKLINE]
- 7 ☐ [Proportionate Mortality Study of Golf Course Superintendents](#)
Kross BC ; Burmeister LF ; Ogilvie LK ; Fuortes LJ ; Mei Fu C
American Journal of Industrial Medicine, Vol. 29, No. 5, pages 501-506, 45 references, 1996 [NIOSH]



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brain cancer pesticides

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Item 1 of 63

Pesticide Prioritization for a Brain Cancer Case-Control Study

Authors:

Sanderson WT
Talaska G
Zaebst D
Davis-King K
Calvert G

Source: Environmental Research, Vol. 74, No. 2, pages 133-144, 28 references, 1997

Abstract:

Procedures used to select pesticides to be included in a NIOSH case control study examining the risk of brain cancer in farm workers in Iowa, Michigan, Minnesota, and Wisconsin associated with pesticide use and other environmental exposures was discussed. A procedure to identify and prioritize the pesticides most appropriate for the study was needed because of the large number and variety of pesticides available, approximately 24,000 commercially registered pesticides, therefore making it impossible to investigate them all. Lists of pesticides were created to document those used in the four states and in the US as a whole utilizing data from the US Department of Agriculture and the departments of agriculture and land grant colleges in each state. Pesticides were then prioritized according to the criteria: volume of use before 1985, ranking of use in the four states and the US as a whole according to pesticide type, and toxicologic evidence of carcinogenic, teratogenic, and mutagenic effects. The criterion 'pesticide use before 1985' was chosen to allow a latency period of at least 10 years for brain cancer. The study was to be based on brain cancer cases diagnosed in the four states from 1985 on. A total of 240 pesticides were used in the four states: 102 herbicides, 81 insecticides, 32 fumigants, and 35 fungicides. Using the criteria above, the list was reduced to 56 herbicides, 49 insecticides, 17 fumigants, and 12 fungicides. The final list represented more than 99% of the total pounds of herbicides and insecticides and more than 99% of the total

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pounds of fungicides and fumigants used in the states before 1985. Lists of the priority **pesticides** are to be sent to the study participants before the study questionnaire is administered to allow them time to recall details of their including specific years of use and crops they were used on. The authors conclude that the procedures used to select the **pesticides** to be examined in this study are useful for documenting past **pesticide** use.

Keywords:

DCN-241835
NIOSH Author
Agricultural chemicals
Occupational exposure
Epidemiology
Brain tumors
Risk analysis
Information systems
Agricultural workers

Coden:

ENVRAL

Entry Month: October, 1998

Year of Publication: 1997

Secondary Source ID: NIOSH00241410

Search PubMed for brain cancer pesticides AND Tox[sb] Go Clear

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1: [Navas-Acien A, Pollan M, Gustavsson P, Floderus B, Plato N, Dosemeci M](#)

[Related Articles, Links](#)

Interactive effect of chemical substances and occupational electromagnetic field exposure on the risk of gliomas and meningiomas in Swedish men.

Cancer Epidemiol Biomarkers Prev. 2002 Dec;11(12):1678-83.
PMID: 12496061 [PubMed - in process]

2: [Stephans SE, Miller GW, Levey AI, Greenamyre JT](#)

[Related Articles, Links](#)

Acute mitochondrial and chronic toxicological effects of 1-methyl-4-phenylpyridinium in human neuroblastoma cells.

Neurotoxicology. 2002 Oct;23(4-5):569-80.
PMID: 12428729 [PubMed - indexed for MEDLINE]

3: [Marikovsky M](#)

[Related Articles, Links](#)

Thiram inhibits angiogenesis and slows the development of experimental tumours in mice.

Br J Cancer. 2002 Mar 4;86(5):779-87.
PMID: 11875743 [PubMed - indexed for MEDLINE]

4: [Slaughter MR, Thakkar H, O'Brien PJ](#)

[Related Articles, Links](#)

Effect of diquat on the antioxidant system and cell growth in human neuroblastoma cells.

Toxicol Appl Pharmacol. 2002 Jan 15;178(2):63-70.
PMID: 11814326 [PubMed - indexed for MEDLINE]

5: [Maeda K, Gotoh H, Chikui E, Furusawa T](#)


[Related Articles, Links](#)

Intratumoral hemorrhage from a posterior fossa tumor after cardiac valve surgery--case report.

Neurol Med Chir (Tokyo). 2001 Nov;41(11):548-50.
PMID: 11758708 [PubMed - indexed for MEDLINE]

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Search fields:

☐ TOXLINE Special

☒ All fields

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☐ Titles

☒ Both New Default

☐ Authors (e.g., Smith H)

Search: ☐ exact words ☒ singular & plural forms
☐ word variants

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25000

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Year of Publication:

1900

through

2003

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BIOSIS

CIS

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DART

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Afrikaans

Arabic

Armenian

Azerbaijani

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Select Record Reference

- ☐ **Beryllium and Beryllium Compounds**
Anonymous
TA: Concise International Chemical Dictionary
YR.2001 IP: VI:32 [RISKLINE]
- ☐ **Beryllium and beryllium compounds**
Anonymous
TA: IARC Monographs on the evaluation of the carcinogenic risk of chemicals to humans PG.41-117
- ☐ **A study on the beryllium lymphocyte transformation test and the beryllium levels in working environment**
YOSHIDA T; SHIMA S; NAGAO H; MORITA K
INDUSTRIAL HEALTH; 35(3): 1997
- ☐ **A study on the beryllium lymphocyte transformation test and the beryllium levels in the working environment**
Yoshida T; et al
Industrial Health July 1997, Vol.35, No.3, p.374-379. 18 ref. [CIS]
- ☐ **Pulmonary function in beryllium workers: Assessment of exposure**
Kriebel D; Sprince NL; Eisen EA; Greaves IA
British Journal of Industrial Medicine Feb. 1988, Vol.45, No.2, p.83-92. Illus. 22 ref. [CIS]
- ☐ **Epidemiology of beryllium sensitization and disease in nuclear workers.**
KREISS K; MROZ MM; ZHEN B; MARTYNY JW; NEWMAN LS
AMERICAN REVIEW OF RESPIRATORY DISEASE; 48(4 PART 1): 1993. 985-991. [BIOSIS]

Save Checked Items
Sort
Details
History
Download
Modify Search
Basic Search
Browse Index
Help
TOXNET Home

Microsoft Internet Explorer provided by National Institutes of Health

Favorites Tools Help

PubMed National Library of Medicine

Nucleotide Protein Genome Structure PMC Taxonomy OMIM Books

for

☒ Limits [Preview/Index](#) [History](#) [Clipboard](#) [Details](#)

Limits: Toxicology

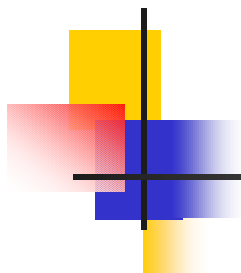
Display Show: Sort Send to

Items 1-20 of 106 of 6 [Next](#)

☐ **1: Taylor TP, Ding M, Ehler DS, Foreman TM, Kaszuba JP, Sauer NN.** [Related Articles, Links](#)
Beryllium in the environment: a review.
 J Environ Sci Health Part A Tox Hazard Subst Environ Eng. 2003 Feb;38(2):439-69.
 PMID: 12638707 [PubMed - in process]

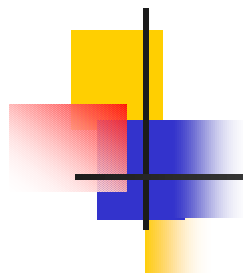
☐ **2: McCanlies EC, Kreiss K, Andrew M, Weston A.** [Related Articles, Links](#)
HLA-DPB1 and chronic beryllium disease: a HuGE review.
 Am J Epidemiol. 2003 Mar 1;157(5):388-98. Review.
 PMID: 12615603 [PubMed - indexed for MEDLINE]

☐ **3: Frome EL, Newman LS, Cragle DL, Colyer SP, Wambach PF.** [Related Articles, Links](#)



Part IV

TRI and other Specialty Files



Toxics Release Inventory (TRI) U.S. Environmental Protection Agency (EPA)

TRI 95-00 – 482,531 Records

- ✍ Facility Identification (Facility Name, Address, Phone, etc.)
- ✍ Substance Identification (Chemical Name, CAS RN, Uses, etc.)
- ✍ Environmental Release of Chemical (in Air, Water, Land, Underground Injection)
- ✍ Waste Treatment
- ✍ Off-Site Waste Treatment
- ✍ Source Reduction and Recycling (Quantity Released, Energy Recovery, Quantity Recycled, Quantity Treated)



TRI Background

- ✍ Right-to-Know Movement – Workplace, Community
- ✍ OSHA Hazard Communication Standard – 1983
- ✍ SUPERFUND = CERCLA (1980)
- ✍ Bhopal (1984) and smaller scale chemical disasters
- ✍ SARA (Superfund Amendments and Reauthorization Act) (1986)
 - ✍ Title 3 = Emergency Planning and Community Right-to-Know Act
 - ✍ Section 313 = Toxic Release Reporting
- ✍ Pollution Prevention Act of 1990

















Search Page - TRI

- ✍ Several search query boxes – fill in any combination.
- ✍ Chemical names or CAS Registry numbers. Let system add synonyms (default) or use exact terms entered.
- ✍ Select Year(s) – 1995-2000
- ✍ Facility Name(s)
- ✍ Facility Location (state, city/state, county/state, zip)
- ✍ Ranging
 - ✍ Greater than _____ pounds
 - ✍ Total Release, Air, Water, Land, Underground Injection
 - ✍ Or “No Release Selected”
- ✍ Browse Index for:
 - ✍ All Words
 - ✍ Chemical Name
 - ✍ CAS Registry Number
 - ✍ Facility Name
 - ✍ Facility City



Search Results Page - TRI

-  Displays facility name, chemical, city/state of retrieved records.
-  Unsorted order
-  Select Record(s) of Interest
-  Calculate Releases – Tabular Display of Total Environmental Releases and Off-Site Waste Transfers for all retrieved records.
-  View Details of Search Strategy
-  Modify Search – Returns you to Search Page with query intact
-  Begin a new Basic Search – Returns you to Search Page with blank query box (note: search screen can't be modified directly from this page)
-  Sort Results – By substance name, facility name, city, or state. Ascending or Descending.
-  Save Checked Items, Display Checked Items
-  View Search History and combine search statements
-  Download – Brief or Full Format
-  Browse Index
-  Get Help
-  Return to TOXNET Home



Selected Record Page - TRI

- ✍ Full record displayed
- ✍ Choose fields for display from Contents (expand, contract categories)
- ✍ Navigate – Next Item, Previous Item
- ✍ View Details of Search Strategy
- ✍ Modify Search – Returns you to Search Screen with query intact
- ✍ Begin a New Search – Returns you to Search Screen with blank query box
- ✍ Browse Index
- ✍ Get Help
- ✍ Download – In Full Format
- ✍ Return to TOXNET Home
- ✍ Link to records for the same chemical in Other Files - (including TOXLINE and ChemID*plus*)



Toxics Release Inventory

[Tox. & Env. Health](#) [TOXNET](#) [TRI](#)

Databases

HSDB	i
IRIS	i
GENE-TOX	i
CCRIS	i
Multi-Databases	i
TOXLINE	i
DART/ETIC	i
Toxics Release Inventory	i
ChemIDplus	i
TOXNET Home	

Search TRI

Other NLM Resources

Chemical Name or CAS Registry Number

methyl ethyl ketone

Search

Clear

Add synonyms and CAS numbers to search:

☒ Yes ☐ No

TRI Files:

☐ 2000 ☒ 1999 ☐ 1998
☐ 1997 ☐ 1996 ☐ 1995

Facility Names

(Separate multiple entries with commas)

Facility Location

(Separate multiple entries for state, city/state, or zip with commas. For example: NJ, DE, or Trenton NJ, Houston TX, or 21113, 21224.)

marshfield/mo

☐ State ☒ City/State
☐ County/State ☐ Zip

Greater Than 0 lbs

for No Release Selected

Search

Browse the Index

[DIRLINE](#)

[Haz-Map](#)

[AltBib](#)

[Tox Weblinks](#)

[MEDLINEplus](#)

[Tox/Env. Health subset](#)

[PubMed](#)

[NLM Gateway](#)

[Locatorplus](#)

Support Pages

[Help](#)

[Fact Sheet](#)

[Sample Record](#)



TRI99 Search Results

[Tox. & Env. Health](#) [TOXNET](#) [TRI99](#)

Calculate
Release!

Save
Checked Items

Sort

Details

History

Download

Modify Search

New Search

Browse Index

Help

TOXNET Home

Please click on **Modify Search** button to modify TRI search strategy.

Items **1** through **2** of **2**

*Facility/Substance Names are **unsorted**.*

Select
Record

Facility/Substance Name

1 ☐

WILCORP INDS. INC.
METHYL ETHYL KETONE
MARSHFIELD, MO

2 ☐

YORK CASKET-MISSOURI
METHYL ETHYL KETONE
MARSHFIELD, MO

TRI99

[Previous Item](#)

[Search Results](#)

[New Search](#)

[Details](#)

[Other Files](#)

[Modify Search](#)

TOXNET
Home

[Download](#)

[Browse Index](#)

[Help](#)

Item 2 of

Contents

Contract all categories ☐

Expand all categories ☐

Select

Clear

- ☐ [FULL RECORD](#)
- ☐ [Facility Identification](#)
- ☐ [Substance Identification](#)
- ☐ [Environmental Release of Chemical](#)
- ☐ [Waste Treatment](#)
- ☐ [Off-Site Waste Transfer](#)
- ☐ [Source Reduction and Recycling](#)
- ☐ [Administrative Information](#)

TRI99

METHYL ETHYL KETONE YORK CASKET-MISSOURI MARSHFIELD, MO

For other data, click on the Table of Contents

Environmental Release of Chemical:

Non-Point Air Emissions Estimates:

Non-Point Air Release: 1,900 lbs./rep yr. 1999

Basis of Estimate: (C) Mass Balance Calculations

Point Air Emissions Estimates:

Point Air Release: 17,000 lbs./rep yr. 1999

Basis of Estimate: (C) Mass Balance Calculations

Total Air Release: 18,900 lbs./rep yr. 1999

Water Discharge Estimates:

Receiving Stream: NA

Water Release: NA

Basis of Estimate: 0%

Total Water Release: 0 lbs./rep yr. 1999

Underground Injection Total: 0 lbs./rep yr. 1999

Land Release Estimates:

Disposal Method: (D03) Land Treatment/Application/Farming

Land Release: NA



Search

as



[Haz-Map Search](#)

[More Searches](#)

[Haz-Map Help](#)

[Glossary](#)

[References](#)

Browse Haz-Map

- **Hazardous Agents**

1. [By Types of Agents](#)
2. [By Adverse Effects](#)
3. [Alphabetically](#)

- **Occupational Diseases**

1. [By Types of Diseases](#)
2. [By Jobs and Symptoms](#)
3. [Alphabetically](#)

- **High Risk Jobs**

1. [By Types of Jobs](#)
2. [Alphabetically](#)

Haz-Map: Information on Hazardous Chemicals and Occupational Diseases
by
Jay A. Brown, M.D., M.P.H.

[Specialized Information Services](#) [U.S. National Library of Medicine](#),

8600 Rockville Pike, Bethesda, MD 20894

[National Institutes of Health](#)

[Privacy/Disclaimer Notice](#)

Customer Service: tehip@tehl.nlm.nih.gov

Last updated: February 14, 2003



Search

as



[Haz-Map Search](#) [More Searches](#) [Haz-Map Help](#) [Glossary](#) [References](#)

Browse Haz-Map by Jobs

[Search TOXNET](#)

Information about this job:

Carpenters

- **High risk job tasks associated with this job:**
 - [Apply arsenic preservatives to wood](#)
 - [Contaminate skin or inhale spray while using pentachlorophenol](#)
 - [Handle agents that cause allergic contact dermatitis or contact urticaria](#)
 - [Installed insulation before 1975](#)
 - [Machine allergenic wood and inhale dust](#)
 - [Remove insulation installed before 1975](#)
 - [Saw or sand arsenic-treated wood](#)
 - [Saw or sand creosote-treated wood](#)
 - [Use epoxy, isocyanate, or formaldehyde-resin adhesives, finishes, or sealants](#)
 - [Use n-hexane as a solvent in glues, coatings, or degreasers](#)
 - [Work with glue solvents](#)



Search as  Agent  Disease  Job  Text Search

[Haz-Map Search](#)

[More Searches](#)

[Haz-Map Help](#)

[Glossary](#)

[References](#)

[Browse Haz-Map](#)

[Search TOXNET](#)

Agent Name	n-Hexane
Alternative Name	Hexane
CAS Number	110-54-3
Formula	C6-H14
Major Category	Solvents
Synonyms	Hexyl hydride, normal-Hexane
Category	Alkanes (Paraffins)
Description	Colorless liquid with a gasoline-like odor;
Sources/Uses	Used as a solvent, especially in the adhesive and shoe industries; abused by glue sniffers for its euphoric effects; [LaDou, p. 371] Used in shoe and furniture manufacture to dissolve glue; also used in adhesive tape manufacturing; [Sullivan, p. 1124]
Comments	n-Hexane is in the list of "Some volatile substances which may be abused by inhalation" published on the web site of the U.N. International Drug Control Programme, indicating its potential to cause narcosis in workers. In addition to CNS solvent syndrome, n-Hexane can cause motor neuropathy.

Exposure Assessment	
<u>BEI</u>	2,5-Hexanedione in urine = 5 mg/g creatinine; end of shift; screen for n-hexane in end-expired air; ACGIH Notice of Intended Change (2001): 2,5-Hexanedione (free) in urine = 4 mg/L end of shift near end of workweek;
<u>Skin Designation (ACGIH)</u>	Yes
<u>TLV (ACGIH)</u>	50 ppm
<u>PEL (OSHA)</u>	500 ppm
<u>IDLH (NIOSH)</u>	1100 ppm
<u>Excerpts from Documentation for IDLHs</u>	It has been reported that a 10-minute exposure to 5,000 ppm caused dizziness and a sensation of giddiness.
<u>Vapor Pressure</u>	124 mm Hg
<u>Odor Threshold Low</u>	65 ppm
<u>Odor Threshold High</u>	248 ppm
<u>Explanatory Notes</u>	IDLH = 10% of LEL (lower explosive limit); Odor threshold from AIHA;
<u>MAK</u>	50 ppm
<u>Half Life</u>	Urine (2,5-hexanedione): 15 hours; blood: 2-3 hours; fat: 64 hours; [TDR, p. 1480]
<u>Reference Link</u>	ATSDR ToxFAQs - n-Hexane
<u>Flammability (NFPA)</u>	3: may ignite at ambient temperature
Adverse Effects	
<u>Neurotoxin</u>	Motor Neuropathy

Household Products Database

[SIS](#) | [NLM](#) | [Help](#)

[Home](#)

[Products](#)

[Ingredients](#)

[Health](#)

Browse & Search

- [Products](#)
- [Ingredients](#)
- [Health Effects](#)

Support Pages

- [About](#)
- [Help](#)
- [Glossary](#)
- [Contact Us](#)
- [Disclaimer](#)
- [Other Resources](#)

[Quick Search](#)

Health & Safety Information on Household Products

What's under your kitchen sink, in your garage, in your bathroom, and on the shelves in your laundry room? Do these household products pose a potential health risk to you and your family?

Find out what's in these products and what are the potential health effects, and other safety and handling information.

[Continue...](#)



[Specialized Information Services](#) [U.S. National Library of Medicine](#),

8600 Rockville Pike, Bethesda, MD 20894

[National Institutes of Health](#)

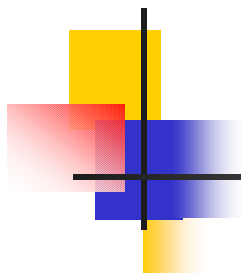
[Privacy/Disclaimer Notice](#)

Customer Service: tehip@tehl.nlm.nih.gov

Last updated: November 5, 2001

PROTOTYPE –

Not Publicly
Accessible Yet



Part V

Non-NLM Resources



Professional Associations

- ✍ Society of Toxicology – <http://www.toxicology.org/>
- ✍ Society of Environmental Toxicology and Chemistry – <http://www.setac.org>
- ✍ American Academy of Clinical Toxicology – <http://www.clintox.org>
- ✍ American Association of Poison Control Centers – <http://www.aapcc.org>
- ✍ Society of Risk Analysis – <http://www.sra.org>
- ✍ Other groups in environmental health, occupational health, industrial hygiene, health physics etc.



U.S. Government Resources

- ✍ Agency for Toxic Substances and Disease Registry (ATSDR) – <http://www.atsdr.cdc.gov>
- ✍ Environmental Protection Agency (EPA) – <http://www.epa.gov>
- ✍ Food and Drug Administration – <http://www.fda.gov>
 - ✍ National Center for Toxicological Research – <http://www.fda.gov/nctr>
- ✍ National Institute for Occupational Safety and Health – <http://www.cdc.gov/niosh>

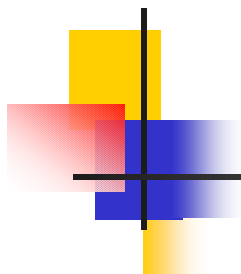


U.S. Government Resources (continued)

- ✍ National Institute of Environmental Health Sciences – <http://www.niehs.nih.gov>
- ✍ National Toxicology Program – <http://ntp-server.niehs.nih.gov>
- ✍ U.S. Chemical Safety and Hazard Investigation Board – <http://www.chemsafety.gov>

Some State Government Sites

- ✍ New Jersey Department of Health and Senior Services – Division of Epidemiology, Environmental and Occupational Health – <http://www.state.nj.us/health/eoh>
- ✍ California – Office of Environmental Health Hazard Assessment – <http://www.oehha.ca.gov>



Some Chemical Databases

- ✍ Chemfinder – <http://www.chemfinder.cambridgesoft.com>
- ✍ International Toxicity Estimates for Risk (ITER) (from TERA) (featuring comparative risk values) – <http://www.tera.org/iter>
- ✍ Scorecard (from Environmental Defense) – <http://www.scorecard.org>
- ✍ Environmental Fate Databases & more (from Syracuse Research Corporation) – <http://esc.syrres.com>
- ✍ EXTOXNET (pesticide information) – <http://ace.orst.edu/info/extoxnet>



Some Chemical Databases (continued)

- ✍ PAN (Pesticide Action Network) Pesticides Database – <http://www.pesticideinfo.org>
- ✍ Where to Find Material Safety Data Sheets on the Internet – <http://www.ilpi.com/msds>
- ✍ RxList, the Internet Drug Index – <http://www.rxlist.com>
- ✍ International Programme for Chemical Safety (IPCS) INCHEM – <http://www.inchem.org/>

Also Consider:

- ✍ Scirus - Elsevier Science - <http://www.scirus.com/>



Other Web Sites

- ✍ UNEP (United Nations Environment Programme) Chemicals – <http://www.chem.unep.ch>
- ✍ Intergovernmental Forum on Chemical Safety - <http://www.who.int/ifcs/>
- ✍ Inter-Organization Programme for the Sound Management of Chemicals - <http://www.who.int/iomc/>
- ✍ National Council for Science and the Environment – <http://www.cnie.org>
- ✍ Society of Environmental Journalists – <http://www.sej.org>
- ✍ TEHIP/NLM Web Links – <http://sis.nlm.nih.gov/Tox/ToxWebLinks.html>



Some Commercial (\$) Databases

- ✍ ARIEL Insight – Ariel Research – <http://www.arielresearch.com>
- ✍ BIOSIS Previews – BIOSIS – <http://www.biosis.org>
- ✍ Chemical Abstracts & CAS Registry – Chemical Abstracts Service – <http://www.cas.org> (also <http://stnweb.cas.org>)
- ✍ CCINFOweb (CHEMINDEX & IPCS/INCHEM are free) – CCOHS – <http://www.ccohs.ca>
- ✍ CIS Database (on occupational health) (from the International Labour Office) (free as a TOXLINE subfile) – <http://www.ilo.org/public/english/protection/safework/cis/products/cisdoc.htm>



Some Commercial (\$) Databases (continued)

- ✍ EMBASE – Elsevier Science – <http://www.embase.com>
- ✍ Environment Abstracts – Congressional Information Service – available from Dialog - <http://www.dialog.com/>
- ✍ MICROMEDEX Databases – MICROMEDEX – <http://www.micromedex.com>
- ✍ Science Direct - Elsevier - <http://www.sciencedirect.com/>
- ✍ Toxicology Abstracts – Cambridge Scientific Abstracts – <http://www.csa.com>
- ✍ Web of Science – ISI – <http://www.isinet.com/>



Some Web Search Engines and Tools

- ✍ AltaVista – <http://www.altavista.com>
- ✍ Google – <http://www.google.com>
- ✍ Hotbot – <http://www.hotbot.com>
- ✍ Yahoo – <http://www.yahoo.com>
- ✍ Meta Search Engines
 - ✍ Go2Net – <http://www.go2net.com>
 - ✍ Dogpile – <http://www.dogpile.com>
 - ✍ Ask Jeeves – <http://www.ask.com>
- ✍ Searchenginewatch – <http://www.searchenginewatch.com>
- ✍ Mailing List Directories – PAML - <http://www.paml.alastra.com/>
CATALIST - <http://www.lsoft.com/lists/listref.html>

TOXNET Exercises

[Note: There is typically more than one “right” approach to answering each of the following questions. Answers, where they are provided, are merely representative, not definitive. Explore.]

TOXICOLOGY DATA FILES

1. What is the CAS registry number and octanol/water partition coefficient of 2,6-dinitrotoluene and what is this chemical used for? [HSDB]

In HSDB, search for **2,6-dinitrotoluene** and click on the 2,6-dinitrotoluene record on the Search Results Page. In the Table of Contents, expand **Chemical/Physical Properties** and click on **Octanol/Water Partition Coefficient**. Expand **Manufacturing/Use Information** and click on **Major Uses**.

2. Has 2,6-dinitrotoluene been shown to be mutagenic in the Ames salmonella test? [HSDB]

MODIFY above search to **2,6-dinitrotoluene ames**, and click on **2,6-dinitrotoluene** record.

3. What is the oral LD50 of caffeine in male rabbits? Also, click on **DETAILS** to view the search strategy. [HSDB]

Search for **oral ld50 caffeine male rabbits** and click on **caffeine** record.

4. Has caffeine been studied as a tumor promoter? Does it cause mutations? [CCRIS, GENE-TOX]

From HSDB caffeine record (above), click on **Other Files**. Select CCRIS. Expand Studies data in Table of Contents and check the boxes for **Tumor Promotion Studies** and **Mutagenicity Studies**. Return to HSDB. Click on **Other Files** again and select GENE-TOX. **Select Mutagenicity Studies**.

5. Which of the toxicology data files contain information on ammonia? What is the Inhalation Reference Concentration (RfC) of ammonia? (Note: the RfC is a non-carcinogenic risk assessment parameter) Also, view the DOWNLOAD options available. [Multi-Data Base and IRIS]

Select the **Multi-Database** option on the TOXNET main page. Search for **ammonia**. Click on the IRIS ammonia record. Expand **Chronic Health Hazard Assessment for Noncarcinogenic Effects** in Table of Contents. Click on **Reference Concentration for Chronic Inhalation Exposure (RfC)**.

TOXNET Exercises (continued)

6. What are some chemicals used in leather tanning and what are their human health effects? [HSDB]

Use the **limits** option of HSDB. Search for **leather tanning** in HSDB. Expand **Manufacturing/Use Information** and check the box for **Major Uses**. Click on several retrieved chemical records to view their “best sections” and click on **Human Health Effects** for these records in the Table of Contents.

7. Does nitrobenzene have any effect on sperm? Find some recent general articles on nitrobenzene. [HSDB, TOXLINE Core]

Search for **nitrobenzene sperm** in HSDB. Click on nitrobenzene record and view **Best Sections**. Click on **Other Files and** click on **TOXLINE Core**.

8. How does the U.S. Environmental Protection Agency characterize the carcinogenicity of methylmercury? [IRIS]

Search for **methylmercury** in IRIS and select the methylmercury record on the Search Results page. Expand category **II. Carcinogenicity Assessment for Lifetime Exposure**. Click on **II.A. Evidence for Human Carcinogenicity**.

9. Find any information on the occurrence or effects of methyl parathion in soil. Search using the chemical's CAS Registry Number – 298-00-0. [HSDB]

Search HSDB for **298-00-0 soil** in the query box and scan the **Best Sections** of the methyl parathion record.

10. Use Boolean operators and phrase searching to look for information on lung cancer or bladder cancer in workers, in HSDB.

Enter – (“**lung cancer**” [htox] OR “**bladder cancer**” [htox]) AND worker

TOXNET Exercises (continued)

TOXICOLOGY LITERATURE FILES

1. Search TOXLINE Special for articles by C.N. Pope. Sort retrieval by primary author names. [TOXLINE Special]

Search for “pope cn” in query box. On “Search Results” page, click on “SORT” button and sort by author.

2. Search TOXLINE Special and TOXLINE Core for phosphoric acid. Explore navigating through your retrieval, examining individual records, and going to linked records. [TOXLINE Special & Core]

Search for **phosphoric acid** in query box. Click on **Details** buttons in both databases to view the respective search strategies. Navigate the pages. Click on records of interest and on hot-linked data – e.g. keywords, author names, CAS registry numbers. Check for related records.

3. Find articles focused on the effects of diet on breast cancer. [TOXLINE Special & Core]

Try a **Limits** search. Enter **diet breast cancer** in the query box. Limit to **Titles**. Select **Both** TOXLINE Special and TOXLINE Core.

4. Find journal references on the treatment of arthritis by the anti-inflammatory agent Celebrex. [TOXLINE Core]

Search for **arthritis celebrex** in the query box. Select the TOXLINE Core radio button.

5. Use the EMIC subfile to determine whether peppermint been tested for mutagenicity. Check for English language articles. [TOXLINE Special]

Conduct a Limits search. Select EMIC as a TOXLINE Component and English as a language from the drop down menus. Enter **peppermint** in the query box.

6. Find information on the effects of alcohol on the fetus. [DART Special and DART Core]

Select **Both** DART Special and DART CORE. Search for **alcohol fetus** in the query box.

TOXNET Exercises (continued)

7. Search TOXLINE Core directly on PubMed to find articles on toxicological aspects of jellyfish. Search for articles published from 2000-2003 in English. [TOXLINE Core via PubMed directly].

Go to PubMed at <http://pubmed.gov>. Click on **Limits**. Enter **jellyfish** in the search query box. Limit the search to the toxicology subfile, the publication dates to 2000-2003 and the language to English.

8. Find information on renal failure associated with amanita mushroom poisoning. Look for English language articles published from 1995 to 2003. [TOXLINE Special]

Conduct a Limits search. Enter **amanita renal failure** in the query box. Restrict publication years to 1995-2003. Select English from the dropdown menu.

9. Use the HISTORY feature to look for hospital or medical waste incineration in TOXLINE Special. [TOXLINE Special]

First search for **“hospital waste” incinerat***. (Using quotes looks for the terms together as a phrase. The asterisk is for truncation and searches for words such as incinerate, incineration, etc.) Then search for **“medical waste” incinerat***. Press the HISTORY button and combine your two searches according to the instructions, and using an “OR” operator.

TOXIC CHEMICAL RELEASES

1. How much ammonia was released to the air and water in Milwaukee in 1999?

In TRI99, search for **ammonia** in the “chemical name” query box and for **Milwaukee/WI** in the “facility location (city/state)” query box. Click on “Calculate Releases.”

2. How much of the above releases came from Red Star Yeast and in what body of water did this facility discharge ammonia?

After above search, go back to the “TRI Search Results” screen. Click on the Red Star Yeast record. Click on “Environmental Release of Chemical” in the Table of Contents. Scroll down to “Water Discharge Estimates.”

TOXNET Exercises (continued)

3. What chemicals have been released to the air, in amounts greater than 100,000 pounds, over Old Hickory, Tennessee in 1995 and 1996? By what companies?

Search for **Old Hickory Tennessee** in the “facility location (city/state)” query box. Select **greater than 100,000 pounds** for “total air release.” Results page will display chemicals and companies.

4. Did Hewlett-Packard’s Newark, California facility transfer any 1,2,4-trichlorobenzene off-site for treatment in 1996? How much? Where to?

In TRI96, search for **1,2,4-trichlorobenzene** in the “chemical” query box, **hewlett-packard** in the “facility name” query box, and **newark california** in the “facility location (city/state)” query box. Click on “Off-Site Waste Transfer” in the Table of Contents.

5. What company has reported the highest underground injection release of a single chemical in 1999? What was the chemical?

In TRI99, select **10,000,000** and “Total Underground Injection” in the “Greater than ____ for ____” drop down menus. For the records retrieved, expand the “Environmental Release of Chemical” category. Click on “Underground Injection Total” for these records and compare the numbers. Identify the chemical with the highest number.

6. How many individual TRI98 reports have been filed on barium compounds?

In TRI98, search **barium compounds** in the chemical query box. Note the number of records retrieved listed at the top of the Search Results page.

HAZ-MAP

1. What are some high risk tasks associated with the job of carpet installation?

Click on **High Risk Jobs** and then on **Carpet Installers**.

TOXNET Exercises (continued)

2. What are some hazards associated with the use of cobalt in the workplace?

Click on **Hazardous Agents**, then on **Cobalt**. Click on **Cobalt** again to view exposure assessment data. Extra – from here highlight some terms and press Search **TOXLINE** to perform a TOXLINE search.

3. What are some hazards of leather tanning?

Perform a “text search” for **leather tanning** in the search query box. Click on **leather tanning and finishing** as an Industry and **tanning leather** as a Process.

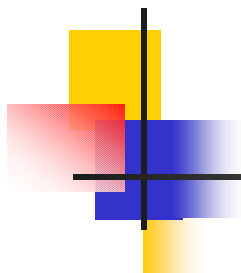
WORLD WIDE WEB

1. Explore EPA’s voluminous Web site, particularly the **Databases and Software** section located by clicking on their home page’s **Information Sources**. Locate IRIS, ECOTOX, the Toxics Release Inventory, and the Safe Drinking Water Information System. Use the Advanced Search box to find documents with **mercury** in the title. [www.epa.gov]
2. Locate a full-text article on why drugs get pulled off the market in the January-February 2002 issue of the **FDA Consumer** magazine. [www.fda.gov]
3. What chemicals are on the list of “Known to be Human Carcinogens” in the National Toxicology Program’s Year 2002 10th Report of Carcinogens? [ntp-server.niehs.nih.gov]
4. Find the Agency for Toxic Substances and Disease Registry’s TOXFAQ profile on nickel. [www.atsdr.cdc.gov]
5. Check out the National Council for Science and the Environment’s Web site and find recent Congressional Research Service (CRS) reports on **pesticides**. [www.cnie.org]
6. Which Florida universities offer graduate programs in toxicology? Check the Society of Toxicology’s Resource Guide to Careers in Toxicology (under Public Outreach/Career Resources) [www.toxicology.org]

TOXNET Exercises (continued)

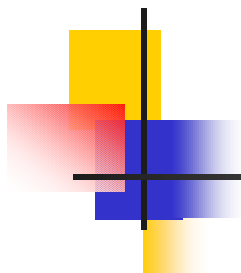
7. Explore the variety of data sources containing information on acrylonitrile, by searching ChemFinder. [www.chemfinder.com]
8. Where and on what dates will the Society of Environmental Toxicology and Chemistry's 2003 Annual Meeting in Europe be held? [www.setac.org]
9. What is New Jersey's rank among states in total release hazardous air pollutants? Use Scorecard (from Environmental Defense). Start by clicking on Pollution Rankings. [www.scorecard.org]
10. How many poison control centers in Texas are certified by the American Association of Poison Control Centers (AAPCC)? What are their addresses? The AAPCC's Poison Center Lists includes a list of certified centers. Find the nation-wide toll-free poisoning emergency phone number. [www.aapcc.org]
11. Use the BIOLOG file (one of Syracuse Research Corporation's Environmental Fate Data Bases - EFDB) to find information about DDT in sewage. [esc.syrres.com]
12. Use the Environmental Journalism site to determine what environmental meetings will be coming up in October 2003. [www.sej.org]
13. How do Health Canada, the U.S. EPA, and ATSDR's evaluations of the noncancer inhalation risk values of styrene compare? [www.tera.org/iter]
14. What are some common side effects of the drug, Vioxx? Consult MEDLINEplus' Drug Information page (data from the USP). [www.nlm.nih.gov/medlineplus/druginformation.html] .

Also consider RxList [www.rxlist.com].
15. Who makes Kill Zone Flea and Tick Killer 2000? What are its active ingredients? How have various governmental agencies rated the carcinogenic potential of these ingredients? [www.pesticideinfo.org]



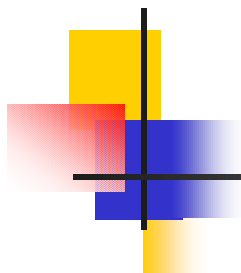
Part VI

ChemID*plus*









ChemID*plus*

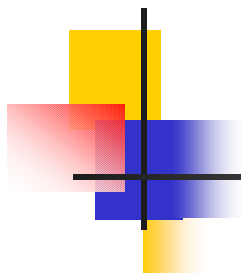
- ✍ Chemical Identification File
- ✍ Chemical Dictionary/Directory File for chemicals cited in MEDLARS Files & outside resources
- ✍ Contains over 365,000 chemical records
- ✍ Structural Data for over 160,000 records
- ✍ Direct Link/Searches of MEDLINE, TOXNET, and other resources







ChemID*plus* Content

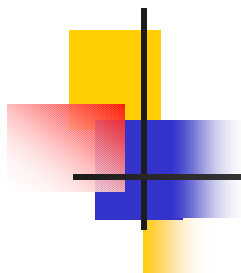
Names and Synonyms

-  **Name of Substance**: Usually the most commonly used name, includes MeSH heading and USAN name
-  **MeSH Heading**: NLM Medical Subject Heading
-  **Systematic Name**: Describes molecular structure
-  **Synonyms**: All other names found for the substance
-  **Mixture Name**: Name of multi-component substance, one of which is the retrieved substance
-  **SUPERLIST names**: The name used by regulatory/guidance lists




ChemID*plus* Content

-  **CAS Registry Number**: Unique number of up to 9 digits assigned by Chemical Abstracts Service used to index chemicals. ChemIDplus uses the hyphenated format
-  **ID**: The ID number is the CAS Registry Number in a non-hyphenated fixed length format or a unique number for entries that have no CAS Registry or NLM assigned numbers
-  **Molecular Structure**: Display of structure (if present) via Chime or ChemSymphony
-  **Registry Numbers**: All CAS Registry Numbers known to be assigned over time to a specific compound



ChemID*plus* Content

 **Formulas**: The molecular formula in a hyphenated format.

 **Classification Codes**: Describe the general category assigned by a given source to a chemical based on toxicity, use and application, pharmacologic and/or therapeutic category, and status on certain chemical lists.

 **Notes**: A textual description of a compound's use and utility, often from MeSH controlled vocabulary.

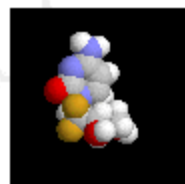
 **Locators**: The names of NLM databases, and other major resources that have information about a given compound, usually hyperlinked.

Division of Specialized Information Services, NLM
ChemIDplus Chemical Search Input Page

A [TOXNET](#) Resource

Welcome to a new and improved
version of ChemIDplus!

New Last Updated: February 2, 2003



ChemIDplus

367369 Records

164073 Structures

Powered by Chemscape TM

<http://www.mdli.com/chemscape>

Data Search Type:

Name/Synonym Equals

MTBE

And optional [Locator Code](#) limit is

Please choose one

[Structure Input Box](#)

The Structure Input Box contains a grid of chemical symbols and a large empty area for drawing structures. The grid includes elements like C, O, N, H, S, P, F, Cl, Br, I, *, and various hydrogen isotopes (H1, H2, H3, H4) and charges (-3, -2, -1, 0, +1, +2, +3). It also features geometric shapes like circles, hexagons, pentagons, squares, and triangles, as well as functional groups like alcohols, amines, and nitriles. The large empty area is surrounded by a toolbar with icons for drawing and editing structures.

Structure Search Type:

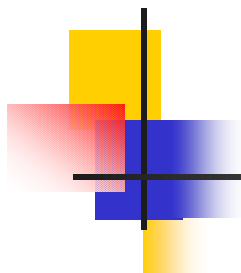
Substructure Search

Display Results

Display chemical structures using

Chime ☐

Java ☒



ChemID*plus* Search Screen

Five drop down menus on the search screen:

- ✎ Data Search Type: Names/Synonym, Registry Number, Formula (hyphenated), Classification Code, Locator Code
- ✎ Logical Operators: Equals (the default), Starts With, Contains
- ✎ Display results: 10 (default), 25
- ✎ Locator Code (optional limit): List of files and locators, MEDLINE, TOXLINE, EPA, FDA, WHO, OSHA, CDC
- ✎ Structure Search Type: Substructure Search, Similarity Search (default 80% similarity), Exact Structure



ChemIDplus

Methyl tert-butyl ether RN: 1634-04-4



[Enlarge Structure](#)

Molecular Structure

Names and Synonyms

Classification Codes

Formulas

Notes

Registry Numbers

Locator Codes

Entire Record

Main Query Page

File Locator

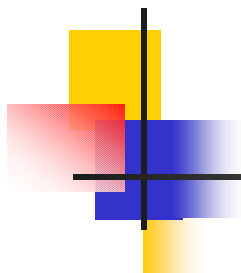
-  [CANCERLIT](#)
-  [CCRIS](#)
-  [DART/ETIC](#)
-  [DSL](#)
-  [EINECS](#)
-  [EMIC](#)
-  [HSDB](#)
-  [Haz-Map](#)
-  [IRIS](#)
-  [MEDLINE](#)
-  [MEDLINEplus](#)
-  [MESH](#)
-  [RTECS](#)
-  [SUPERLIST](#)
-  [TOXLINE Core](#)
-  [TOXLINE Specia](#)
-  [TRI2000](#)
-  [TRI95](#)
-  [TRI96](#)
-  [TRI97](#)
-  [TRI98](#)
-  [TRI99](#)
-  [TSCANV](#)

Welcome to the ChemIDplus Locator Page

The window to the left displays one or more ChemIDplus Locator Codes which link to other sites that carry information about the chemical you have retrieved. You may click on:

- A hyperlinked Locator Code such as [TOXLINE](#) to retrieve data from that resource. Results will be displayed in this window.
- The information icon () to get a description of the source of the Locator Code and the scope of the search.

The window on the top of the screen displays buttons that you may click on to change the data displayed for this chemical or to change your search mode. Hold your mouse pointer over a button to see a more detailed description.



Locator Code Page

- ✍ Hyperlinked locators directly search resources on a substance
- ✍ Information icon (i) next to the locator gives the description of the database and scope



ChemIDplus

Query Results 1 - 2 of 2

Main Query
Page

Options	ID	Structure	CAS	Molecule Name	Formula
Full Record Enlarge Structure Use Structure For Query Use Structure for Similarity	000081072		81-07-2	Saccharin [USAN]	C7-H5-N-O3-S
Full Record Enlarge Structure Use Structure For Query Use Structure for Similarity	000128449		128-44-9	Saccharin sodium anhydrous	C7-H5-N-O3-S.Na



ChemIDplus

Saccharin sodium anhydrous RN: 128-44-9

Molecular
Structure

Names and
Synonyms

Classification
Codes

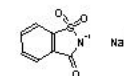
Formulas

Registry
Numbers

Locator
Codes

Entire
Record

Main Query
Page



[Enlarge Structure](#)

File Locator

[i CCRIS](#)
[i DART/ETIC](#)
[i DSL](#)
[i EINECS](#)
[i EMIC](#)
[i GENETOX](#)
[i RTECS](#)
[i SUPERLIST](#)
[i TOXLINE](#)
[i TOXLINE Special](#)
[i TSCAINV](#)

Internet Locators

[i EPA CRS](#)

Superlist Locator

[i CA65](#)
[i HPV](#)
[i IARC](#)
[i INER](#)
[i MA](#)
[i PA](#)
[i PAFA](#)

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[ChemIDplus](#)

Zidovudine [USAN:BAN:INN:JAN] RN: 30516-87-1

[Molecular
Structure](#)

[Names and
Synonyms](#)

[Classification
Codes](#)

[Formulas](#)

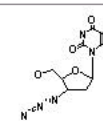
[Notes](#)

[Registry
Numbers](#)

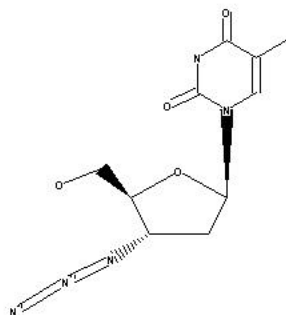
[Locator
Codes](#)

[Entire
Record](#)

[Main Query
Page](#)



[Enlarge
Structure](#)



ID:
030516871

CAS Number:
30516-87-1

[Enlarge
Structure](#)
[Use Structure
For Query](#)
[Use Structure
for Similarity](#)

Formula:
C10-H13-N5-O4

**Names and
Synonyms**

MeSH Heading

- Zidovudine

Mixture Name

- Combivir
- Trizivir

Name of Substance

- Zidovudine
- Zidovudine [USAN:BAN:INN:JAN]

Superlist Name

- 3'-Azido-3'-deoxythymidine
- Zidovudine

Synonyms

- (component of) Combivir
- (component of) Trizivir
- 1-(3-Azido-2,3-dideoxy-beta-D-ribofuranosyl)-5-methylpyrimidine-2,4-(1H,3H)-dione
- 3'-Azido-3'-deoxythymidine
- AZT
- Azidothymidine
- BW A509U
- BW-A 509U
- CCRIS 105
- Compound S
- DRG-0004
- HSDB 6515
- NSC 602670
- Retrovir
- ZDV
- Zidovudina [Spanish]
- Zidovudine
- Zidovudinum [Latin]

Systematic Name

- Azidothymidine
- Thymidine, 3'-azido-3'-deoxy-

Classification Codes	<u>Classification Code</u> <ul style="list-style-type: none"> • Anti-HIV agents • Antimetabolites • Antimetabolites, antineoplastic • Antiretroviral • Antiviral • Drug / Therapeutic Agent • Human Data • Mutation data • Reproductive Effect • Reverse transcriptase inhibitors • Tumor data
Formulas	<u>Superlist Classification Code</u> <ul style="list-style-type: none"> • Overall Carcinogenic Evaluation: 2B
Locators	<u>Molecular Formula</u> <ul style="list-style-type: none"> • C10-H13-N5-O4 <u>File Locator</u> <ul style="list-style-type: none"> • AIDS DRUGS • AIDS LINE • CANCER LIT • CCRIS • ClinicalTrials.gov • DART/ETIC • DSL • EMIC • HSDB • MEDLINE • MEDLINEplus • MESH • MESH HEADING • RTECS • SUPERLIST • TOXLINE • TOXLINE Core • TOXLINE Special

Notes

Registry Numbers

Internet Locators

- NIAID ChemDB
- NIAID HIV DRUGS
- healthfinder

Superlist Locator

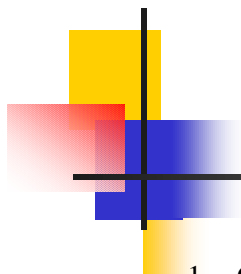
- IARC
- NTPT

Note

- A dideoxynucleoside compound in which the 3'-hydroxy group on the sugar moiety has been replaced by an azido group. This modification prevents the formation of phosphodiester linkages which are needed for the completion of nucleic acid chains. The compound is a potent inhibitor of HIV replication, acting as a chain-terminator of viral DNA during reverse transcription. It improves immunologic function, partially reverses the HIV-induced neurological dysfunction, and improves certain other clinical abnormalities associated with AIDS. Its principal toxic effect is dose-dependent suppression of bone marrow, resulting in anemia and leukopenia.

CAS Registry Number

- 30516-87-1



ChemIDplus Exercises

1. Check the file locator to see what NLM databases contain information on phenytoin. Search DART without leaving ChemIDplus.

Type Phenytoin in search box, click Search. Click DART/ETIC in left pane under File Locator, view record in right pane.

2. Locate the record for styrene and link to the Internet Locator ATSDR TOXFAQS. Next link to the NIOSH Pocket Guide. Is styrene on the EPA Clean Air Act (CAA1)? Activate the Classification Code button and find the IARC classification on carcinogenicity, click on the "i" to see the source.

Type styrene in the search box, click Search. Scroll down the left pane and under Internet Locators click the link to ATSDR TOXFAQs. Next, scroll down and under Superlist Locator click the link to the CAA1 listing for styrene. At the top of the screen, click the button for Classification Code. Under Superlist Classification Code, click the "i" for Overall Carcinogenic Evaluation..... to view this source in the right pane.

3. Find the "valium" record in ChemIDplus and use its structure to do substructure and similarity searches respectively. How many structures are in each category?

Type valium in the search box, click Search. Now click the Molecular Structure button at the top. Click Use Structure for Query button. Choose Similarity Search from the Structure Search Type pull-down list and click Search. Type in a percent similarity between 50 and 100, the default is 80 percent, but you may have to use a lower number if you don't retrieve any hits. For a substructure search, go back to the Structure Search page (click back button on your browser), choose Substructure Search from the Structure Search Type pull-down list, click Search

4. Identify all the HSDB records that are ozone depletors (CAA2).

Choose Locator Code from the Data Search Type pull-down list. Type HSDB in the search box. In the pull-down list that says "and optional Locator Code limit is" choose CAA2 from the pull-down list. Click Search.